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Semiclassical propagator to evaluate off-diagonal matrix elements of the evolution operator between quantum states

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We present a powerful semiclassical expression to evaluate off-diagonal matrix elements of the evolution operator between quantum states constructed in the neighborhood of unstable short periodic orbits, which is valid up to the Heisenberg time. The expression is much easier to evaluate than the Van Vleck propagator and consists of a sum over the set of heteroclinic orbits, where each term of the series is computed by canonical invariants. Here we introduce relevant canonical invariants of heteroclinic orbits and with them at hand, the semiclassical expression is derived. Finally, our formula is successfully verified in the hyperbola billiard.

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Introduction. Semiclassical propagation of waves is a fruitful approach to understand and evaluate a wide set of physical processes in atomic and molecular systems. Nevertheless, long-time propagation in Hamiltonian systems with classically chaotic dynamics is a long-standing unsolved problem, the main reason being that the Van Vleck propagator [1] suffers from serious drawbacks. Specifically, the evolution operator in configuration space $\langle q''|e^{-i\hat{H}t/\hbar}|q'\rangle$ [2] is evaluated by the method of semiclassical propagation [3,4] as follows. The state $|q''\rangle$ is associated with the plane $(q = q'', p)$ in phase space and the state $e^{-i\hat{H}t/\hbar}|q'\rangle$ with the classical evolution (for a time t) of the plane $(q = q', p)$; these planes and their evolutions are Lagrangian manifolds [5,6]. Then it is necessary to compute the set of submanifolds resulting from the intersection of $(q = q'', p)$ and the evolution of $(q = q', p)$. This is a hard geometrical problem and moreover the calculation must be repeated for all times involved.

Recently, we showed that by using the stable and unstable manifolds of periodic orbits it is possible to achieve long-time propagation [7,8]; these manifolds are Lagrangian manifolds existing on a surface of constant energy and so they are time invariant. The idea is to construct a quantum state $|\gamma\rangle$ in the neighborhood of a short periodic orbit γ [9], which is represented in phase space by a tube enclosing γ. Then the forward and backward evolutions take place by stretching the tube along the unstable and stable manifolds. Consequently, the ket and bra of the diagonal matrix element $(\langle\gamma|e^{-i\hat{H}t/2\hbar})(e^{-i\hat{H}t/2\hbar}|\gamma\rangle)$ are associated with the unstable and stable manifolds, respectively. In this way, the geometrical problem is enormously simplified because the intersection of these manifolds consists of the set of homoclinic orbits of γ. However, as the required classical information is huge because each homoclinic orbit is infinite, it is mandatory to express the corresponding semiclassical contribution in terms of canonical invariants. In this respect, we have found four relevant canonical invariants to compute $\langle\gamma|e^{-i\hat{H}t/\hbar}|\gamma\rangle$ [7,10]: the homoclinic action S, the homoclinic Maslov index μ, the relevance A, and the normalized Lazutkin invariant L.

In this Rapid Communication we obtain a semiclassical expression to evaluate the off-diagonal matrix element $\langle\delta|e^{-i\hat{H}t/\hbar}|\gamma\rangle$ valid for long times of the order of the Heisenberg time; δ is a short periodic orbit different from γ. This matrix element is given by a sum over the set of heteroclinic orbits (HEOs) connecting γ and δ and each term of the series is evaluated by four canonical invariants. We first introduce the canonical invariants used and later derive the semiclassical expression. Finally, the formula is verified in the hyperbola billiard [11].

Notation. Given a two degrees of freedom chaotic Hamiltonian system, let us consider a Poincaré surface of section where the dynamics is specified by the map M. Moreover, γ and δ are given by the fixed points z_γ and z_δ on the section [12], with the stable ξ_s and unstable ξ_u manifold directions at the fixed points normalized by $\xi_u^\gamma \wedge \xi_s^\gamma = \xi_u^\delta \wedge \xi_s^\delta = 1$.

Let us parametrize the manifolds of z_γ as follows. The forward evolution by κ steps of a point on the unstable direction $z = M^\kappa(z_\gamma + \varepsilon\xi_u^\gamma)$ exists on the unstable manifold $\mathscr{M}_u^\gamma$ of γ ($|\varepsilon| \ll 1$). One associates z with $u_\gamma = |\varepsilon| e^{\kappa P_\gamma \lambda_\gamma} + O(\varepsilon^2)$, where P_γ is the period of γ and λ_γ its stability index, and gets the vector $\xi_u^\gamma(z) = dz/du_\gamma$ tangent to $\mathscr{M}_u^\gamma$ at z. In contrast, the backward evolution of a point on the stable direction $z = M^{-\kappa}(z_\gamma + \varepsilon\xi_s^\gamma)$ exists on the stable manifold $\mathscr{M}_s^\gamma$ of γ and by using the parametrization $s_\gamma = |\varepsilon| e^{\kappa P_\gamma \lambda_\gamma} + O(\varepsilon^2)$ of z one gets the vector $\xi_s^\gamma(z) = dz/ds_\gamma$ tangent to $\mathscr{M}_s^\gamma$ at z. Of course, the manifolds of z_δ are parametrized in the same way by using the period P_δ of δ and its stability index λ_δ.

Let ζ be a HEO going from γ to δ (γ is the starting orbit and δ is the ending one), which is defined on the section by the infinite sequence of points $\ldots, z_{-1}, z_0, z_1, \ldots$, with $M z_n = z_{n+1}$; that is, $\lim_{n\to-\infty} z_n = z_\gamma$ and $\lim_{n\to+\infty} z_n = z_\delta$. Moreover, ζ' is a HEO going from δ to γ, which is defined by the sequence $\ldots, z'_{-1}, z'_0, z'_1, \ldots$.

Heteroclinic stability. This is a canonical invariant associated with each HEO. For ζ it is evaluated at an arbitrary z_n by

$$D = u_\gamma(z_n)\xi_u^\gamma(z_n) \wedge s_\delta(z_n)\xi_s^\delta(z_n), \tag{1}$$

where the starting (ending) orbit uses the unstable (stable) manifold. This is independent of the selected surface of section and reduces to the product AL when γ and δ are the same orbit, with A the homoclinic relevance and L the Lazutzin.

Heteroclinic relevance. This canonical invariant, related to the pair (ζ, ζ'), is evaluated at arbitrary points z_n and z'_m by

$$\tilde{A} = [\tilde{u}_\gamma(z_n)\tilde{s}_\gamma(z'_m)]^{\lambda_\delta/(\lambda_\gamma+\lambda_\delta)}[\tilde{u}_\delta(z'_m)\tilde{s}_\delta(z_n)]^{\lambda_\gamma/(\lambda_\gamma+\lambda_\delta)}. \tag{2}$$

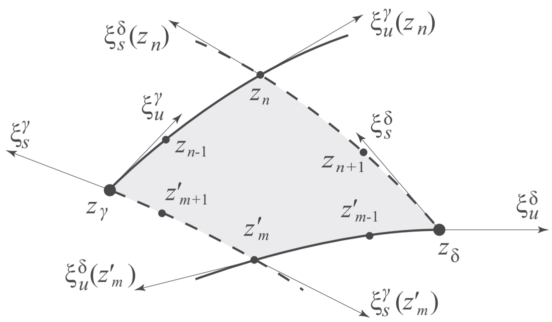

FIG. 1. Closed circuit defined by the selected points z_n and z'_m corresponding to two heteroclinic orbits between z_γ and z_δ.

The tilde indicates another parametrization of the manifolds [13] given by (equivalent relations work at z'_m)

$$\tilde{u}_\gamma(z_n) = u_\gamma(z_n)\exp\left(\lambda_\gamma \sum_{i=-\infty}^{n-1}(t_i - P_\gamma)\right),$$

$$\tilde{s}_\delta(z_n) = s_\delta(z_n)\exp\left(\lambda_\delta \sum_{i=n}^{+\infty}(t_i - P_\delta)\right),$$

with t_i the time for going from z_i to z_{i+1}; the sums converge because $(t_i - P_\gamma)$ $[(t_i - P_\delta)]$ goes exponentially to zero as $i \to -\infty$ $(i \to +\infty)$. This invariant is independent of the selected surface of section.

Heteroclinic action. This canonical invariant depends on the selected points z_n and z'_m used to define a closed circuit on the surface of section. For instance, the closed circuit displayed in Fig. 1 defines the symplectic area $S(z_n,z'_m)$ (shadowed area in the figure), which is evaluated by

$$\sum_{i=-\infty}^{n-1}(S_i - S_\gamma) + \sum_{i=n}^{+\infty}(S_i - S_\delta) + \sum_{i=-\infty}^{m-1}(S'_i - S_\delta) + \sum_{i=m}^{+\infty}(S'_i - S_\gamma),$$

with S_i (S'_i) the action for going from z_i to z_{i+1} (z'_i to z'_{i+1}) and S_γ (S_δ) the action of γ (δ). The four sums correspond to the following paths: from z_γ to z_n along $\mathscr{M}_u^\gamma$, from z_n to z_δ along $\mathscr{M}_s^\delta$, from z_δ to z'_m along $\mathscr{M}_u^\delta$, and from z'_m to z_γ along $\mathscr{M}_s^\gamma$. It is trivial to verify the relations $S(z_n,z'_m) = S(z_{n-1},z'_{m-1}) = S(z_{n-1},z'_m) - \Delta S = S(z_n,z'_{m-1}) + \Delta S$, where $\Delta S = S_\gamma - S_\delta$.

Heteroclinic winding number. This invariant is defined in the same way as the heteroclinic action. The closed circuit displayed in Fig. 1 defines an integer number of half turns of the manifold directions $\mu(z_n,z'_m)$ evaluated by the expression

$$\sum_{i=-\infty}^{n-1}(\mu_i - \mu_\gamma) + \sum_{i=n}^{+\infty}(\mu_i - \mu_\delta) + \sum_{i=-\infty}^{m-1}(\mu'_i - \mu_\delta) + \sum_{i=m}^{+\infty}(\mu'_i - \mu_\gamma).$$

Here μ_i (μ'_i) is the angle swept by the unstable manifold direction as we move from z_i to z_{i+1} (z'_i to z'_{i+1}), divided by π, and μ_γ (μ_δ) is the winding number of γ (δ). In particular, for the closed circuit of the figure $\mu(z_n,z'_m) = 0$. Moreover, one has $\mu(z_n,z'_m) = \mu(z_{n-1},z'_{m-1}) = \mu(z_{n-1},z'_m) - \Delta\mu = \mu(z_n,z'_{m-1}) + \Delta\mu$, where $\Delta\mu = \mu_\gamma - \mu_\delta$.

Assigning invariants to individual heteroclinic orbits. We use the following criteria.

(i) It is easy to verify that the sequence

$$d_n = \ln[u_\gamma(z_n)/s_\delta(z_n)]/(P_\gamma\lambda_\gamma + P_\delta\lambda_\delta)$$

satisfies $d_n = 1 + d_{n-1}$. Then one takes n such that $0 \leqslant d_n < 1$ and selects the points z_{n-1} and z_n with probabilities d_n and $1 - d_n$, respectively [14].

(ii) Let ζ_0 (ζ'_0) be the HEO from γ to δ (δ to γ) with the smallest $|D|$ and then select [according to (i)] the point $z_a \in \zeta_0$ $(z'_a \in \zeta'_0)$ with the greatest probability. These HEOs define the simplest transitions between γ and δ and so we assume that they are equivalent (for instance, see Fig. 1). Specifically, given $S_0 = S(z_a,z'_a)$ [for this circuit $\mu(z_a,z'_a) = 0$], we assign to each path (one from γ to δ through z_a and the other from δ to γ through z'_a) an action $S_0/2$, a winding number 0, and a relevance $\tilde{A}_0$, with $\tilde{A}_0$ the relevance of the pair (ζ_0,ζ'_0).

(iii) We assign to ζ the relevance

$$A = \tilde{A}^2/\tilde{A}_0,$$

with $\tilde{A}$ the relevance of the pair (ζ,ζ'_0). Furthermore, we only use two paths from γ to δ. The path going through z_n has heteroclinic action and winding number

$$S = S(z_n,z'_a) - S_0/2, \quad \mu = \mu(z_n,z'_a)$$

and we assign to this path the probability $1 - d_n$. The other path (with probability d_n) goes through z_{n-1} and has action and winding number $S + \Delta S$ and $\mu + \Delta\mu$.

Heteroclinic Maslov index. When the system includes hard walls, it is necessary to add the contribution by boundary conditions at the walls as follows:

$$\tilde{\mu} = \mu + \sum_{i=-\infty}^{n-1}(N_i - N_\gamma) + \sum_{i=n}^{+\infty}(N_i - N_\delta),$$

with N_i the number of bounces (with the walls) satisfying Dirichlet condition minus the number satisfying Neumann condition, when one goes from z_i to z_{i+1}; the same applies for N_γ (N_δ) along γ (δ). Of course, $\tilde{\mu}_\gamma = \mu_\gamma + N_\gamma$ $(\tilde{\mu}_\delta = \mu_\delta + N_\delta)$ is the Maslov index of γ (δ), while $\Delta\tilde{\mu} = \Delta\mu + N_\gamma - N_\delta$.

The states $|\gamma\rangle$ *and* $|\delta\rangle$. Here $|\gamma\rangle$ has n_γ excitations along γ and mean energy $\langle\gamma|\hat{H}|\gamma\rangle = E_\gamma + O(\hbar^{3/2})$, with E_γ satisfying

$$S_\gamma/\hbar - \tilde{\mu}_\gamma\pi/2 = 2\pi n_\gamma; \tag{3}$$

the dispersion is $\sqrt{\langle\gamma|(\hat{H} - E_\gamma)^2|\gamma\rangle} = \hbar\lambda_\gamma/\sqrt{2} + O(\hbar^{3/2})$ [15]. The same applies for $|\delta\rangle$ with n_δ excitations and Bohr-Sommerfeld energy E_δ. The state $|\gamma\rangle$ has a simple representation in configuration space by using local coordinates on γ [9,15]. The so-called resonance is the product of a local plane wave along γ and a transverse wave packet that evolves according to a modified dynamics (we eliminate the contraction-expansion contribution to the motion in the vicinity of γ). After one turn around γ the wave packet accumulates the phase $S_\gamma/\hbar - \tilde{\mu}_\gamma\pi/2$, which is an integer multiple of 2π when the energy is E_γ [see (3)]. To have some intuition, with q and p the variables on the Poincaré section, the restriction of $|\gamma\rangle$ to the section is given by

$$\frac{e^{i\varphi_\gamma}}{\left[\pi\hbar P_\gamma^2\left(q_u^2+q_s^2\right)\right]^{1/4}}\exp\left[-\frac{(q-q_\gamma)^2}{2\hbar}\Gamma+\frac{i}{\hbar}p_\gamma(q-q_\gamma)\right],$$

with $\Gamma=(p_u+ip_s)/(q_u+iq_s)$, $(q_u,p_u)=\xi_u^\gamma$, $(q_s,p_s)=\xi_s^\gamma$, and $(q_\gamma,p_\gamma)=z_\gamma$.

Semiclassical correlation. We compute the correlation by

$$\langle\delta|e^{i(E-\hat{H})t/\hbar}|\gamma\rangle=(\langle\delta|e^{i(E_\delta-\hat{H})t_\delta/\hbar})(e^{i(E_\gamma-\hat{H})t_\gamma/\hbar}|\gamma\rangle),$$

where the ket (bra) is a forward (backward) propagation of $|\gamma\rangle$ ($\langle\delta|$) for a time t_γ (t_δ). Here $t_\gamma=(1-\varepsilon)t/2$ and $t_\delta=(1+\varepsilon)t/2$, with ε being in principle arbitrary, and [16]

$$E=(E_\gamma+E_\delta)/2-\varepsilon(E_\gamma-E_\delta)/2. \quad (4)$$

At a semiclassical level, the ket (bra) is a WKB state existing on $\mathscr{M}_u^\gamma$ ($\mathscr{M}_s^\delta$) and so the contribution of ζ results in

$$e^{i(\varphi_\gamma-\varphi_\delta)}\sqrt{2\pi\hbar}F_0(t)\overline{e^{i\alpha}},$$

where $\varphi_\gamma-\varphi_\delta$ is the phase difference between the initial states on the Poincaré section and $\overline{e^{i\alpha}}=(1-d_n)e^{i\alpha}+d_ne^{i(\alpha+\Delta\alpha)}$ is the mean phase over the selected paths, with $\alpha=S/\hbar-\tilde{\mu}\pi/2$ and $\Delta\alpha=\Delta S/\hbar-\Delta\tilde{\mu}\pi/2$. In contrast, $F_0(t)$ computes at time t the accumulated contribution to the amplitude

$$F_0(t)=\int_{-\infty}^{\infty}\frac{\Phi_s[z(t'),-t_\delta]\Phi_u[z(t'),t_\gamma]}{\left|\xi_u^\gamma[z(t')]\wedge\xi_s^\delta[z(t')]\right|^{1/2}}e^{i(E_\gamma-E_\delta)t'/\hbar}dt', \quad (5)$$

where $z(t')$ runs over ζ at energy E [17]. Here Φ_u (Φ_s) is the amplitude of the ket (bra) on $\mathscr{M}_u^\gamma$ ($\mathscr{M}_s^\delta$) [7],

$$\Phi_u[z(t'),t_\gamma]=\frac{1}{P_\gamma^{1/2}(\pi\hbar)^{1/4}}\exp\left[-\frac{A}{2\hbar}e^{2\lambda_\gamma(t'-t_\gamma)}-\lambda_\gamma t_\gamma/2\right],$$

$$\Phi_s[z(t'),-t_\delta]=\frac{1}{P_\delta^{1/2}(\pi\hbar)^{1/4}}\exp\left[-\frac{A}{2\hbar}e^{-2\lambda_\delta(t'+t_\delta)}-\lambda_\delta t_\delta/2\right],$$

and $\xi_u^\gamma[z(t')]\wedge\xi_s^\delta[z(t')]=e^{(\lambda_\delta-\lambda_\gamma)t'}D/A$. The imaginary exponential in (5) is included because the expression for Φ_u (Φ_s) is valid for ζ at energy E_γ (E_δ); specifically, $(E_\gamma-E_\delta)t'$ is the action (as we move along ζ) at E_γ minus the action at E_δ.

By the change of variable $y=\bar{\lambda}t'$ in (5), with $\bar{\lambda}=(\lambda_\gamma+\lambda_\delta)/2$, and defining the dimensionless parameters [18]

$$\varepsilon=(\lambda_\gamma-\lambda_\delta)/2\bar{\lambda},\quad \eta=(E_\gamma-E_\delta)/2\bar{\lambda}\hbar,$$

the semiclassical correlation for $0\leqslant t<\tau$ results in

$$\langle\delta|e^{i(E-\hat{H})t/\hbar}|\gamma\rangle\simeq\frac{\sqrt{\hbar}e^{i(\varphi_\gamma-\varphi_\delta)}}{\bar{\lambda}(P_\gamma P_\delta)^{1/2}}\sum_{t_A\lesssim\tau}\frac{f_\eta^\varepsilon[\lambda(t-t_A)]}{\sqrt{|D|}}\overline{e^{i\alpha}}. \quad (6)$$

The sum runs over the set of HEOs from γ to δ, with

$$\lambda=(1-\varepsilon^2)\bar{\lambda},\quad t_A=\ln(A/\hbar)/\lambda, \quad (7)$$

and the switching function (it starts to be relevant for $x>0$)

$$f_\eta^\varepsilon(x)=\sqrt{2}e^{-x/2}\int_{-\infty}^{\infty}\exp[-e^{2\varepsilon y-x}\cosh(2y)+(\varepsilon+i2\eta)y]dy.$$

The integral can be expanded in powers of ε by using $K_\nu(x)=\int_0^\infty e^{-x\cosh(t)}\cosh(\nu t)dt$, the modified Bessel function of order ν [19]; $f_\eta^\varepsilon(x)=\sqrt{2}e^{-x/2}[K_{i\eta}(e^{-x})+O(\varepsilon)]$ [see Fig. 2(a)] [20].

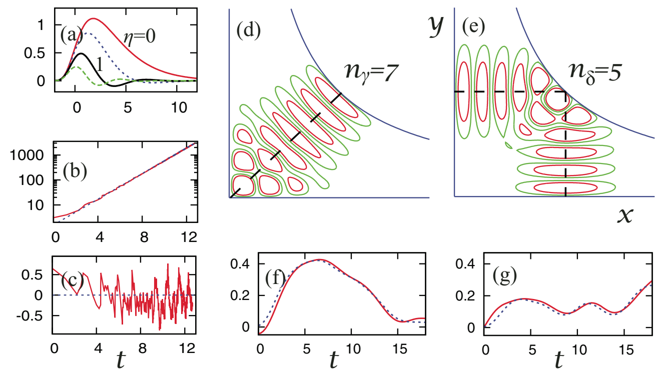

FIG. 2. (Color online) (a) Switching function $f_\eta^\varepsilon(x)$ for $\varepsilon=0$ and $\eta=0,0.5,1,1.5$. (b) Plot of $N(t)$ (solid line) and $\overline{N(t)}$ (dashed line). (c) Plot of $(N-\overline{N})/\sqrt{N}$. (d) Periodic orbit γ (dashed line) in the hyperbola billiard and contour lines at 1 and 0.2 of the probability density of a resonance of γ. (e) Same as (d) but for δ. (f) Real part of the quantum (solid line) and semiclassical (dashed line) correlation between the states of (d) and (e). (g) Same as (f) but for the imaginary part.

Note that (6) results independently of d_n for $E_\gamma=E_\delta$ because in such a case $\Delta\alpha=2\pi(n_\gamma-n_\delta)$ [see (3)].

Heteroclinic orbits. In order to verify (6) we consider the hyperbola billiard, a strongly chaotic Hamiltonian system consisting of the free motion of a particle, with mass and speed taken as unity, within the region $0\leqslant y\leqslant 1/x$ of the Euclidean plane. The shortest periodic orbit is named γ and the next one δ (see Fig. 2), with $P_\gamma=2\sqrt{2}$, $P_\delta=4$, $\lambda_\delta=\ln(3+\sqrt{8})/2$, and $\lambda_\gamma=\lambda_\delta/\sqrt{2}$. In Ref. [8] we found $\mathscr{M}_u^\gamma$, given by an infinity set of disjoint curves on the Poincaré section. Here $\mathscr{M}_s^\delta$ is obtained in a similar way, while the intersection of $\mathscr{M}_u^\gamma$ and $\mathscr{M}_s^\delta$ provides the set of HEOs from γ to δ.

As the semiclassical time t_A [see (7)] indicates when the heteroclinic contribution starts to be relevant, the set of HEOs is ordered by increasing values of A (t_A is the transition time through the HEO). We find 1427 HEOs with relevance $A<A_c=10\,000$; HEOs connected by symmetry were included only once (each HEO is connected by reflection in the diagonal $x=y$ with the other one).

In order to analyze the convergence of (6) we define the excursion time of a HEO (a classical time) by

$$\tilde{t}_A=\ln(A/\sqrt{A_\gamma A_\delta})/\lambda, \quad (8)$$

with $A_\gamma\approx 0.953$ ($A_\delta\approx 0.960$) the relevance of the first homoclinic orbit of γ (δ). Then we study $N(t)$, the number of HEOs with excursion time smaller than t. This function increases exponentially and fluctuates around the mean value $\overline{N(t)}=ae^{bt}$, with $a\approx 1.586$ and $b\approx 0.591$. Figure 2(b) displays $N(t)$ and $\overline{N(t)}$ and Fig. 2(c) shows the fluctuation. According to this result, the sum over heteroclinic contributions in (6) is at most conditionally convergent. In contrast, by assuming no correlation among different heteroclinic contributions, the convergence is guaranteed because $b/\lambda\approx 0.809<1$. Notice that b is the same as that obtained for homoclinic orbits [8] and also is close to the topological entropy $h \approx 0.592$ given in Ref. [21]. These facts suggest that $\overline{N(t)} \sim e^{ht}$ is always valid.

Numerical results. Reference [8] provides the expression for the resonance of γ and [13] gives the one of δ. Figures 2(d) and 2(e) display resonances of γ and δ, while Figs. 2(f) and 2(g) show the correlation between them for a long time (the Ehrenfest time is around 2 and the Heisenberg time is 42). At a semiclassical level we use the obtained set of HEOs in (6), where $\tau \sim \ln(A_c/\hbar)/\lambda$. As it can be seen, the semiclassical approximation provides a good estimate; the error is computed by the mean value $E_r = (1/\tau)\int_0^\tau |C_Q(t) - C_S(t)|dt \approx 0.025$, with C_Q and C_S the quantum and semiclassical correlations, respectively. Moreover, we have computed E_r for other values of n_γ and n_δ, finding an error that is well estimated by $3.3k^{-3/2}$, with k the wave number at the energy given by (4); this expression was obtained in Ref. [8] to estimate the error of diagonal matrix elements.

Conclusion. A HEO contributes to the correlation when a point $\varepsilon_u \xi_u^\gamma$ of the HEO evolves into the point $\varepsilon_s \xi_s^\delta$, with ε_u and ε_s $O(\sqrt{\hbar})$. This transition occurs for a time $t \simeq t_A$ and consists of three stages clearly identified by the relation $t_A \approx t_E^\gamma + \tilde{t}_A + t_E^\delta$, with $t_E^\gamma = \ln(A_\gamma/\hbar)/2\lambda_\gamma$ the Ehrenfest time of $|\gamma\rangle$ (the same applies for t_E^δ). First, the point $\varepsilon_u \xi_u^\gamma$ goes away from the vicinity of γ after the time t_E^γ, then the evolved point makes an excursion for a time $\tilde{t}_A$, and finally it goes to the vicinity of δ. Within this scheme, a direct transition is characterized by $\tilde{t}_A \lesssim 0$.

The expression for λ [see (7)] was derived from (6) by requiring the same time dependence for all HEOs to minus a shift. Furthermore, from the definition of the excursion time [see (8)], which uses λ, one obtains that the number of HEOs with $\tilde{t}_A$ smaller than t is $\sim e^{ht}$ (h is the topological entropy). This is surprising because we obtain an expression for λ that works at a classical level from a semiclassical derivation.

Finding homoclinic and heteroclinic orbits with a long excursion time is much easier than periodic orbits with a long period. In the first case, the search is reduced to the intersection of two well defined curves on a Poincaré section, while in the second case the search covers the full section. For this reason, it should be interesting to develop semiclassical expressions equivalent to the Gutzwiller formula [1] in terms of homoclinic and heteroclinic orbits; a first step in such a direction was given in Ref. [7]. We would also like to mention the interesting use of homoclinic orbits developed in Ref. [22] to characterize properties of scarring.

The obtained matrix elements, just the off diagonal of this Rapid Communication or the diagonal of Ref. [7], have a relative error $O(\hbar)$ in correspondence with the used approximation.

The obtained accuracy is limited to Hamiltonian systems without traces of integrability (see the discussion of Ref. [8]). The extension of our development to systems with mixed dynamics requires an understanding of the influence of small stable regions on the structure of manifolds.

Equation (5) shows clearly the enormous advantage of using canonical invariants. See the Supplemental Material [13] to clarify the evaluation of (5).

The evolution of resonances is given by $\langle x,y|\hat{I}e^{-i\hat{H}t/\hbar}|i\rangle$, with $\hat{I}$ the identity operator in the basis of resonances. Let $\{\langle x,y|i\rangle\}$ be a set of N resonances of the shortest periodic orbits, with Bohr-Sommerfeld energies existing in an energy window of width $\Delta E \gtrsim \hbar\lambda_L$ (λ_L is the Lyapunov exponent). By construction $\langle i|i\rangle = 1 + O(\hbar)$ and we select $N \simeq \rho\Delta E$, where ρ is the mean energy density [9]. Then, with $\langle i|j\rangle = O(\sqrt{\hbar})$ [Eq. (6) at $t = 0$], one can use for practical purposes $\hat{I} \approx \sum_i a_i |i\rangle\langle i| - \sum_{i\neq j}\langle i|j\rangle|i\rangle\langle j|$, where $a_i = \sum_j |\langle i|j\rangle|^2$.

The basis of resonances is particularly efficient to propagate waves existing in a narrow energy window. This often occurs when a system is affected by a moderated perturbation.

With the off-diagonal matrix elements of this Rapid Communication, plus the diagonal ones of Ref. [7], it is possible to propagate quantum waves for long times of the order of the Heisenberg time. This result elucidates a long-standing unsolved problem and probably encourages the development of asymptotic techniques for similar processes, for instance, the propagation of acoustic or electromagnetic waves in complex media.

Acknowledgment. This work was partially supported by CONICET.

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[13] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevE.89.020901 to clarify the parametrization of Eq. (2) and the evaluation of Eq. (5). Also, the expression for the resonance of δ is given.
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[16] Note that $t = t_\gamma + t_\delta$ and $Et = E_\gamma t_\gamma + E_\delta t_\delta$.
[17] We select z at $t' = 0$ by the condition $\tilde{u}_\gamma(z) = \tilde{s}_\delta(z) = \sqrt{A}$.

[18] Here $|\varepsilon| < 1$ and $|\eta| \lesssim 1$ according to the dispersion of the states.

[19] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, DC, 1972).

[20] With $\tilde{K}_\nu(x) = \partial K_\nu(x)/\partial \nu$ and $\tilde{K}'_\nu(x) = d\tilde{K}_\nu(x)/dx$, one has $O(\varepsilon) = \varepsilon[\tilde{K}_{i\eta}(e^{-x})/2 + e^{-x}\tilde{K}'_{i\eta}(e^{-x})]$.

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